

^{35}Cl NQR Studies of Hydrogen Transfer in Crystalline *p*-Chlorobenzoic Acid

Taka-aki Nihei, Shin'ichi Ishimaru, and Ryuichi Ikeda

Department of Chemistry, University of Tsukuba, Tsukuba 305-8571, Japan

Reprint requests to Prof. R. I.; Fax: +8 12 98 53 65 03; E-mail: ikeda@staff.chem.tsukuba.ac.jp.

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^{35}Cl NQR frequencies and spin-lattice relaxation times T_{1Q} were measured in *p*-ClC₆H₄CO₂H (PCBA) and *p*-ClC₆H₄CO₂D (PCBA-*d*₁) at 77–333 K. T_{1Q} in PCBA gave a shallow minimum of 8.0 ms at ca. 110 K, which could be explained by a double proton transfer mechanism in the carboxylic acid dimer referring to ^1H NMR data giving a T_{1H} minimum at almost the same temperature. PCBA-*d*₁ showed temperature dependent NQR frequencies quite analogous to those in PCBA, whereas their T_{1Q} behaviour was quite different in its minimum value and its temperature as well as temperature gradient. These results were explained by suppressed deuteron tunnelling and the Ubbelohde effect.

Key words: Cl NQR; Hydrogen-Bond; Hydrogen-transfer; Tunneling.